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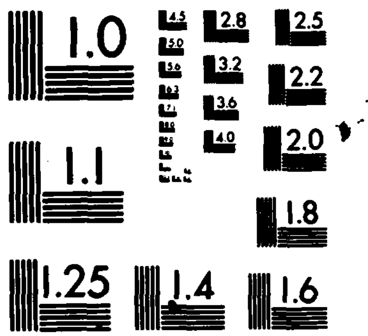

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INVESTIGATIONS OF THE INTERACTIONS OF RADIATION WITH MATTER

FINAL REPORT

STEVEN T. MANSON

JULY 31, 1986

U.S. ARMY RESEARCH OFFICE

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GEORGIA STATE UNIVERSITY

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Work on the interaction of radiation with matter is described. In particular charged particle impact ionization of atoms and molecules is discussed, along with photoabsorption by excited states and ground state atoms, and properties of atomic ions. ~~The~~ relevance of ~~the~~ research to applications in radiation damage and protection, nuclear pumped and x-ray lasers, IR generation and detection, and atmospheric beam devices is pointed out.

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During the period of this contract from the U.S. Army Research Office, our theoretical research in atomic and molecular physics has proceeded apace. In this report, our major areas of investigation are discussed with the progress made in each area highlighted. Also discussed is the applicability of the research areas to various Army needs, where applicable. The report is as non-technical as possible; ample references are given to published works where the technical details can be found. In addition, a complete listing of the 31 publications resulting from this work is presented as an appendix.

I. IONIZATION BY CHARGED PARTICLE IMPACT

The range and energy loss of charged particles passing through matter is related to the ionization of the matter by the charged particles. Hence a knowledge of the ionization probability, i.e., cross section, is the principal constituent of calculations of radiation shielding and damage of both men and materials. Furthermore, the passage of an ion or neutral particle beam through the atmosphere (or any medium) is limited in penetration by inelastic collisions, primarily ionization.

Another important application is in the possibility of a nuclear-pumped laser where the energy from fission fragments is transferred to a lasing medium. Ionization cross sections of the medium constituents, along with the spectrum of secondary electrons which cause further excitations and ionization, are of critical importance in modelling the nuclear-pumped laser situation. In a related context, ionization cross sections of

atoms by charged particle impact is relevant to the possibility of creating population inversions necessary to the working of an x-ray laser.

Thus ionization cross sections, of interest in a variety of applications, are needed. Many of those required are either unobtainable at the present level of experiment, or simply unavailable, thereby pointing out the need for theoretical estimates.

Our work has dealt with total cross sections, single differential cross sections (SDCS) or energy distribution of secondary electrons, double differential cross sections (DDCS) or energy and angular distribution of secondary electrons and multiple ionization cross sections. The total and SDCS are the primary results needed as input for the applied area, but the DDCS and multiple ionization cross sections are necessary to elucidate ionization mechanisms and to fully assess the validity of the calculational work.

One major project in this area has been to develop a semi-empirical model of SDCS which can be used to extend existing data. This model, based on the Bethe asymptotic form of the Born approximation, uses optical data which is more generally available than charged particle data. It has been quite successful in predicting the SDCS for ionization of atoms and molecules by protons and electrons.[1-4] We have also tackled the problem of ionization by ions which carry their own electrons; the general theory has been worked out[5] and we are presently attempting to apply it.

At the more fundamental level, our work has proceeded in two different directions. First, we have been studying multiple ionization which, although relatively small for light atoms, dominates for the heavier ones. Our work[6-9] has been concerned with elucidating the mechanisms that lead to multiple ionization. In one case[7], we have discovered that the previous ideas of how multiple ionization took place were entirely incorrect; a process thought to be very rare actually dominates the double ionization of neon.

In addition, we have delved into the DDCS for ion-atom collisions where the projectile brings in its own electrons[10-12] in an effort to understand all of the processes which lead to secondary electron emission. This work, in collaboration with an experimental group, has shown the importance of the simultaneous ionization of projectile and target.[12] This is very unexpected for high energy collisions and is causing us to re-examine the dynamics of such collisions.

Finally, in this area, we have made a study of inner shell ionization of light atoms by electrons with applications to analytic electron microscopy in mind.[13] This study was presented in such a manner so that the results can be adapted to the experimental conditions of each particular instrument.

II. RELATIVISTIC EFFECTS IN PHOTOABSORPTION OF HEAVY ELEMENTS

Photoabsorption by heavy elements in the UV and x-ray range is of importance in the area of radiation physics generally, and specifically in the areas of radiation protection and shielding

of personnel and materials. While the situation is fairly well-understood for light elements, for heavy elements the situation is otherwise.

We have embarked upon a study of photoionization cross sections for high-Z atoms. This theoretical study was performed within the framework of the explicitly relativistic Dirac equation so as to incorporate the relativistic interactions a priori and not as perturbations.

A major focus in this study has been the relativistic effects on the most sensitive feature of the ionization probability (cross section), the point at which they are zero, known as Cooper minima.[14] These minima are pervasive throughout the periodic table[15] and profoundly affect the cross sections. Relativistic interactions split a single minimum into three. Our work has shown that this splitting can be huge.[16-19] This result was originally found in relatively simple calculations, but we have performed much more sophisticated calculations which confirm it. The minima have a significant effect on photoelectron angular distributions, which are of importance in connection with radiation transport and the deposition of energy in biological tissue; they also affect branching ratios, which are of importance in such areas of isotope separation of heavy atoms (like uranium).

We have also been trying to unravel the various types of relativistic effects in photoionization.[20] The attempt here is to understand which aspect(s) of relativity are important in photoionization and which can be ignored. Basically, this effort

has been to ascertain the crucial interactions that must be included in a calculation to obtain quantitative accuracy.

III. PHOTOABSORPTION BY EXCITED STATES

Excited states of atoms are produced in quantity in hot environments, such as in the vicinity of an atmospheric thermonuclear blast; thus their properties are of interest. In addition, a detector in the IR range, with a quantum efficiency of unity, is now possible using lasers to excite atoms to states with ionization potentials in the IR range. Therefore, photoabsorption cross sections for excited atomic states are required.

In previous work,[21,22] the general systematics of excited state photoionization emerged, along with a great profusion of minima (not present for ground states) which lead to transmission windows. Our investigations have been aimed at looking deeper into these minima[23-26] by looking at new situations, and using more sophisticated calculations. Among this work was a major study on discrete and ionizing transitions for a number of excited states of the cesium atom.[26]

We have also endeavored to compare with experiment wherever possible. For sodium, one measurement showed excellent agreement with our calculations,[27] and another seemed to validate the existence of these new minima[28] and also showed agreement with our calculations.

IV. PROPERTIES OF ATOMIC IONS

Positive ions are also produced in any very hot environment, as discussed above. Their properties are, therefore, of interest in this connection as well as in connection with the passage of a possible x-ray laser beam through the atmosphere.

Properties of atomic ions can be related to a small set of key parameters. One of these properties, the phase shift (or quantum defect) has been studied for all atomic ions for the first 37 members of the periodic table.[29,30] This study has shown the systematics of changes as one goes to higher and higher stages of ionization; that the rich chemical differences of the neutral atoms rapidly disappear.[29] We have also found that our calculational method gave excellent agreement with experiment in the limited number of cases where experiment exists.[29] This led us to produce a tabulation of the results.[30]

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